

OPTIMIZED LAGRANGIAN APPROXIMATIONS FOR MODELLING LARGE-SCALE STRUCTURE AT NON-LINEAR STAGES

by

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Summary: We report on a series of tests of Newtonian Lagrangian perturbation schemes using N-body simulations for various power-spectra with scale-independent indices in the range -3 to $+1$. The models have been evolved deeply into the non-linear regime of structure formation in order to probe the dynamical and statistical performance of the Lagrangian perturbation schemes (whose first-order solution contains as a subset the celebrated “Zel’dovich-approximation” (hereafter ZA). These tests reveal properties of the approximations at stages beyond the obvious validity of perturbation theory. Recently, another series of tests of different analytical and semi-numerical approximations for large-scale structure was conducted with the result that ZA displays the best dynamical performance in comparison with the N-body simulations, if the initial data were smoothed before evolving the model, i.e., a truncated form of ZA (TZA). We show in this Letter that the excellent performance of TZA can be further improved by going to second order in the Lagrangian perturbation approach. The truncated second-order Lagrangian scheme provides a useful improvement over TZA especially for negative power indices, which suggests it will be very useful for modelling standard scenarios such as “Cold-”, “Hot-” and “Mixed-Dark-Matter”.

1. Lagrangian perturbation theory put into perspective

Zel'dovich (1970, 1973) proposed an approximation (hereafter ZA) by extrapolating the Eulerian linear theory of gravitational instability into the non-linear regime using the Lagrangian picture of continuum mechanics. He discussed interesting consequences of this approximation which is capable of describing shell-crossing singularities which, in this model, develop into highly anisotropic oblate “pancake” structures. Those structures can be fundamentally understood and classified in the framework of the Lagrange-singularity-theory, (Arnol'd *et al.* 1982, Shandarin and Zel'dovich 1989, Roshansky *et al.* 1994 and references therein). Zel'dovich's work initiated many applications making it one of the most cited articles in astronomy; it emerged as a standard tool to model principal elements of the large-scale structure, is used to initialize most N-body codes employed by the cosmology community, and forms the basis of more sophisticated approximations like the adhesion approximation (Gurbatov *et al.* 1989, Kofman *et al.* 1992). Zel'dovich's model can be derived by formulating the Euler-Poisson system in terms of Lagrangian coordinates and solving the Lagrangian evolution equations for the field of trajectories perturbatively (Buchert and Götz 1987, Buchert 1989, 1992). It appears as a subclass of the irrotational Lagrangian first-order solution which covers substantial non-linearities in contrast to the Eulerian first-order solution. This explains the success of this approximation if applied to non-linear gravitational structure formation (compare Coles *et al.* 1993).

The particular justification that ZA could be relevant to hierarchical clustering has developed slowly (Melott *et al.* 1983; Melott and Shandarin 1990; Kofman 1991; Little *et al.* 1991; Kofman *et al.* 1992; Coles *et al.* 1993; however see Peebles 1993). A general consensus is forming based around a unification of the former Soviet (“pancake”) and Western (hierarchical clustering) theories.

The Lagrangian theory of gravitational instability is now used in large-scale structure modelling much as the Eulerian theory of gravitational instability used to be. Numerous efforts concern the investigation and application of Lagrangian perturbation solutions up to the third order (Buchert 1989, 1992, Moutarde *et al.* 1991, Bouchet *et al.* 1992, Buchert 1993, Buchert and Ehlers 1993, Gramann 1993, Giavalisco *et al.* 1993, Lachièze-Rey 1993a,b, Buchert 1994, Juszkiewicz *et al.* 1994, Bernardeau 1994, Munshi and Starobinsky 1994, Munshi *et al.* 1994), and, most recently, the investigation of general relativistic analogues (which are intrinsically Lagrangian in the eigensystem of the flow) (Matarrese *et al.* 1993, Kasai 1993, Croudace *et al.* 1994, Bertschinger and Jain 1994, Matarrese *et al.* 1994a,b, Bertschinger and Hamilton 1994, Kofman and Pogosyan 1994, Salopek *et al.* 1994).

2. Optimization of Lagrangian perturbation schemes

Until recently, ZA was evolved only until shell-crossing, i.e., when singularities in the density field develop, at the epoch when the Eulerian representation of the basic dynamical equations breaks down. In principle, the Lagrangian representation of the flow allows following the evolution across caustics, where the flow field itself remains finite. This implies neglecting self-gravitating interaction of multi-stream systems developing inside caustics, however, secondary generations of shell-crossings can be modelled as observed in N-body simulations by going to higher orders in the perturbation approach (Buchert and Ehlers 1993). Melott *et al.* 1994a (hereafter MPS) investigated the performance of a new approximation which requires truncation of high frequencies in the initial power-spectrum before evolving ZA (hereafter: TZA) taking the evolution of large-scale structure deeply into the non-linear regime. MPS found that filtering the initial data with a Gaussian at a scale close to but smaller than the non-linearity scale yields the best agreement with the density fields of the same (untruncated) initial data as evolved by an N-body code.

The non-linearity scale k_{nl} is defined by:

$$a^2(t) \int_0^{k_{nl}(t)} d^3k \mathcal{P}(k) = 1 \quad , \quad (1)$$

where $k_{nl}(t)$ is decreasing with time as successively larger scales enter the non-linear regime; $a(t)$ is the scale factor of the homogeneous background ($a(t_i) \equiv 1$), and $\mathcal{P}(k)$ denotes the initial power-spectrum taken to be a powerlaw with indices in the range -3 to $+1$.

“Best agreement” was defined in terms of an optimal scale k_{opt} in k -space at which the usual cross-correlation coefficient S between the resulting density fields attains its maximum:

$$S := \frac{\langle \delta_1 \delta_2 \rangle}{\sigma_1 \sigma_2} \quad , \quad (2)$$

where $\delta_\ell, \ell = 1, 2$ represent the density contrasts in the analytical and the numerical approximations, respectively, $\sigma_\ell = \sqrt{\langle \delta_\ell^2 \rangle - \langle \delta_\ell \rangle^2}$ is the standard deviation in a Gaussian random field; averages $\langle \dots \rangle$ are taken over the entire distribution. We believe this is the most important statistical test, because it measures whether the approximation is moving mass to the right place, with an emphasis on dense regions. We also allow for small errors by calculating S for the two density arrays smoothed at a variety of smoothing lengths.

For the Lagrangian perturbation schemes up to the third order which were used in our tests see (Buchert 1994). We conducted several tests: In the first step we studied “pancake

models”, i.e., models which a priori have a truncated power-spectrum, in order to study principal effects of a second- and higher-order correction to ZA (for details see Buchert *et al.* 1994a). In the second step we analyzed the whole family of models with powerlaw-spectra $-3, \dots, +1$ by evolving them deeply into the non-linear regime (for details see Melott *et al.* 1994b). These “hierarchical models” have been evolved for expansion factors of 240 to 5100, depending on spectral index and k_{nl} .

Besides the cross-correlation coefficient (3) as a function of scale, we analyzed several statistics including the comparison of the evolved power-spectrum, the evolved r.m.s. values of the density contrast as a function of scale, the phase-angle accuracy achieved by the analytical models, and the evolved density distribution functions.

For all these statistics and for all spectra studied with different filter types and filter scales, we always found improvement for the second-order scheme upon first-order (TZA), if the initial data are truncated with a *Gaussian filter* at a slightly larger scale k_{opt} than the scale needed for the optimal TZA.

In Fig. 1 we display slices of the final density fields for the spectrum with index $n = -1$ as calculated by the N-body code and the first- and second-order Lagrangian approximations at the stage where the non-linearity scale has evolved to $k_{nl} = 8k_f$; k_f is the fundamental mode of the simulation box.

In Fig. 2 we present the results of the most important statistical test which probes the dynamics of the models, i.e., the cross-correlation coefficient (3) for the whole family of hierarchical models at the same evolution stage.

Considerably more details can be found in Melott *et al.* (1994b), where we show more statistical tests applied for the range of indices $-3 \leq n \leq 1$.

3. Conclusions

We summarize our main conclusions and list the advantages of going to second-order in perturbation theory for the purpose of modelling highly non-linear stages:

- 1. The statistics which probe the gravitational dynamics of the models show improvement due to second-order corrections. This success is found for a considerably higher non-linearity than expected from a perturbation approach.
- 2. The improvement (although minor for much small-scale power) is *robust* by going to later stages and to smaller scales. This holds for any spectrum and for any statistics analyzed.
- 3. The CPU times on a CRAY YMP are for the first-order scheme 25 seconds, and for the second-order scheme 60 seconds; the corresponding CPU times on a CONVEX C220 are 2 and 5 minutes. Thus, even the second-order scheme is competitive with *one step* in a corresponding PM-type N-body simulation.
- 4. The high speed as well as the fact that the second-order scheme is as easy to implement as the first-order scheme (directly from the initial data), render this model suitable for all areas of application where thus far ZA was used, e.g., the initialization of N-body codes.
- 5. The second-order scheme predicts much faster collapse of first objects (treating also tidal effects) at times comparable to the collapse time in the widely used spherical “tophat” model (Moutarde *et al.* 1991, Buchert and Ehlers 1993, Munshi *et al.* 1994). Thus, it is preferred for the treatment of ensembles of collapsing objects and for normalization purposes.
- 6. Since the second-order corrections to TZA provide noticeable improvement of dynamical accuracy for initial data with negative sloped power-spectra, we expect that the truncated second-order scheme will be especially useful for the modelling of standard cosmogonies (like Hot-, Cold-, and Mixed-Dark-Matter).
- 7. This modelling will be effective for large sample calculations, since in numerical realizations of ‘fair’ samples in excess of $300 \text{ h}^{-1} \text{ Mpc}$, performed with the same resolution as the simulations reported here (128^3 particles on 128^3 meshes), the truncation scale is close to the Nyquist frequency of the N-body computing. Thus, shortcomings of the analytical schemes become negligible which puts them in an ideal position for the purpose of simulating the environment of galaxy formation down to scales where other physical effects start to affect models based on the description of self-gravity alone. Our method can be effective down to galaxy group mass scales ($10^{13} M_{\odot}$), or better if we include biasing or go to epochs earlier than the present. Thus many things which have been studied by

N-body simulation can now be generated by approximation. The code for second-order is available on request from tob @ mpa-garching.mpg.de .

- 8. The third-order scheme does not show the ‘robustness’ observed for second- and first-order. However, to draw definite conclusions the *analytical* solution of the third-order effect must be studied with reduced numerical uncertainties in its realization by Fast-Fourier-Transform, as pursued by Buchert *et al.* (1994b).

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Figure Captions

Figure 1: Thin slices (thickness $L/128$) of the density fields are displayed for the numerical (a), the optimally truncated first-order (b) and second-order (c) approximations for the evolution stage corresponding to $k_{nl} = 8k_f$, and for the single power-spectrum with index $n = -1$. The grey-scale is logarithmic in order to emphasize the high-density regions.

Figure 2: The cross-correlation coefficient S as a function of the standard deviation σ_ρ of the smoothed numerical simulation for the different power-spectra $n = -3, -2, -1, 0, +1$ (Figs. 2a,b,c,d,e). The cross-correlation of the N-body with the optimally truncated first-order model is shown as a dotted line; with the optimally truncated second-order model a dashed line.